3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Information regarding the chemical identity of hydrogen sulfide is located in Table 3-l. This information includes synonyms, chemical formula and structure, and identification numbers.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of hydrogen sulfide is located in Table 3-2.

With regard to the odor threshold for hydrogen sulfide, it should be noted that although odor can be perceived at 0.5 ppb in air, olfactory fatigue can occur at concentrations of 100 ppm or greater causing a loss of odor perception (Leonardos et al. 1969).

TABLE 3-1. Chemical Identity of Hydrogen Sulfide

Characteristic	Information	Reference
Chemical name	Hydrogen sulfide	HSDB 1998
Synonym(s)	Hydrosulfuric acid; stink damp; sulfur hydride; sulfurated hydrogen; dihydrogen monosulfide; dihydrogen sulfide; sewer gas	HSDB 1998
Registered trade name(s)	No data	Budavari et al. 1996; HSDB 1998
Chemical formula	H_2S	OHM/TADS 1998
Chemical structure	H – S – H	HSDB 1998
Identification numbers:		
CAS registry	7783-06-4	HSDB 1998
NIOSH RTECS	MX1225000	RTECS 1998
EPA hazardous waste	U135	HSDB 1998
OHM/TADS	7216752	OHM/TADS 1998
DOT/UN/NA/IMCO shipping	UN1053; IMO 2.1	HSDB 1998
HSDB	576	HSDB 1998
NCI	No data	HSDB 1998

CAS = Chemical Abstracts Service; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

TABLE 3-2. Physical and Chemical Properties of Hydrogen Sulfide

Property	Information	Reference
Molecular weight	34.08	Budavari et al. 1996
Color	Colorless	ACGIH 1991
Physical state	Gas	Budavari et al. 1996
Freezing point	-85.49°C	Budavari et al. 1996
Boiling point	-60.33°C	Budavari et al. 1996
Specific gravity	1.192	ACGIH 1991
Density at 0°C, 760 mmHg:	1.5392 g/L	Budavari et al. 1996
Odor	Characteristic of rotten eggs	Budavari et al. 1996
Odor threshold:		
Water	0.000029 ppm	Amoore and Hautala 1983
Air	0.5 ppb	Leonardos et al. 1969
Solubility:		
Water at 20°C	One gram in 242 mL	Budavari et al. 1996
Organic solvent(s)	Alcohol, ether, glycerol, gasoline, kerosene, crude oil, carbon disulfide	HSDB 1998; Budavari et al. 1996
Partition coefficients:		
Log K_{ow}	Not applicable	
Log K_{oc}	Not applicable	
Vapor pressure at 21.9°C	1929 kPa; 14,469 mmHg	Lide and Frederikse 1993
Acid dissociation:	$H_2S \rightleftharpoons H^+ + HS^-$ (1′); $HS^- \rightleftharpoons H^+ + S^{2-}$ (2′)	Beauchamp et al. 1984; Budavari et al. 1996
pK_a (1')	7.04	
pK_a (2')	11.96	
Henry's law constant:		
at 20°C	468 atm/mole fraction	Al Haddad et al. 1989
at 30°C	600 atm/mole fraction	
at 40°C	729 atm/mole fraction	
Autoignition temperature	500°C	OHM/TADS 1998
Flammability limits	Upper, 46%; lower, 4.3% (by volume at room temperature)	
Conversion factors	1 ppm = 1.40 mg/m^3	NIOSH 1997
Explosive limits	Upper, 46%; lower 4.3% (by volume in air)	Budavari et al. 1996